

Adler-Bell-Jackiw anomaly in Weyl semi-metals: Application to Pyrochlore Iridates

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Weyl semimetals are three dimensional analogs of graphene where the energy of the excitations are a linear function of their momentum. Pyrochlore Iridates ($A_2Ir_2O_7$) with A =yttrium or lanthanide element) are conjectured to be examples of such a system, with the low energy physics described by twenty four Weyl nodes. An intriguing possibility is that these materials provide a physical realization of the Adler-Bell-Jackiw anomaly. In this letter we investigate the properties of pyrochlore iridates in an applied magnetic field. We find that the dispersion of the lowest landau level depends on the direction of the applied magnetic field. As a consequence the magneto-conductivity in an electric field, applied parallel to the magnetic field is highly anisotropic, providing a detectable signature of the semi-metallic state.

Graphene[1] and topological insulators[2–4] have provided the venue for condensed matter realizations of non-trivial phenomena originally in the realm of high energy physics. Massless relativistic fermions[5], Klein tunneling [5], Theta vacuum (i.e. axion electrodynamics) [6], and Majorana modes [6, 7] are a few examples. A common feature of these systems is that the low energy physics is described by a two component Dirac Hamiltonian with the fermionic momentum is confined to two dimensions. Recently pyrochlore iridates have been conjectured to realize the Adler-Bell-Jackiw (ABJ)[8, 9] chiral anomaly, adding another example to the growing list.

Wan et al. [10] explored the possibility of the three dimensional analog of graphene being realized in the pyrochlore iridates. These materials have a large spin orbit couplings and are in a regime of intermediate correlations, making them promising candidates to realize topological insulators[11, 12]. They have a magnetic ground state[13, 14] and, within a LSDA+U+SO calculations, conjectured to be semi-metals. Most strikingly the low energy physics is described by the Weyl equation, which is the two component version of the Dirac equation. There are 24 Weyl nodes, three around each L point ([111] and equivalent directions) in the Brillouin zone (see fig.1). Nodes related either by inversion or reflection about the $\{xy, yz, zx\}$ planes have opposite chirality. Consequently the material is expected to have an anomalous hall response to applied uniaxial pressure and is susceptible to charge ordering in large magnetic fields[15].

In a quantizing magnetic field, the Lowest Landau Level (LLL) is a linear function of the magnitude of a momentum, with the sign determined by the band structure. If an electric field is applied parallel to the magnetic field, the Adler-Bell-Jackiw (ABJ)[8, 9] axial anomaly leads to an anomalous magneto-conductance. The origin of this effect is in the production of Weyl fermions of a given chirality and an equivalent annihilation of the opposite chirality[16]. This translates to a transfer of particles from one Weyl node to another of opposite chirality at a constant rate. To reach a steady state, this is balanced by inter-node scattering due to impurities.

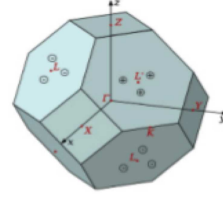


FIG. 1: The low energy physics of pyrochlore iridates is described by linearly dispersing fermionic modes near nodes in the band structure. The position of Weyl nodes in the Brillouin zone is shown in the figure (figure taken from ref[10]). There are three nodes, with the same chirality, located in the vicinity of the L points, and nodes related by inversion have opposite chirality.

In the absence of the magnetic field, the intra-node scattering is quite effective in relaxing the momentum. In the presence of a large field, such that only the LLL is occupied, intra-node scattering is suppressed due to a lack of phase space. The only scattering mechanism available are processes that involve different nodes of opposite chirality. Since these nodes are located at different point in the Brillouin zone, Nielsen and Ninomeya [16] argued that the corresponding scattering rate is much smaller implying a large magneto-conductivity.

In this letter we focus on the anomalous magneto-conductivity expected in Weyl semi-metals [10, 16]. In general the Hamiltonian takes the form $\pm \vec{q} \cdot \mathbf{V} \cdot \vec{\sigma}$ where \vec{q} is the momentum, \mathbf{V} is a real matrix, \pm label right handed (RH) and left handed (LH) chirality, and $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$. We first address the question of the dispersion of the LLL for arbitrary \mathbf{V} . We find that the energy is determined by the component of the momentum parallel to the applied field. Crucially the velocity of the mode also depends on the direction of the magnetic field leading to highly anisotropic response.

The low energy Hamiltonian in the vicinity the Weyl nodes of the proposed topological semimetal state is

$$H(\vec{q}) = \left(\Delta + \frac{q_z^2}{2m_1} - \frac{q_\perp^2}{2m_2} \right) \sigma_z + (\beta q_z + c_1 q_\perp^3 \cos(3\theta)) \sigma_y + c_2 q_\perp^3 \sin(3\theta) \sigma_x \quad (1)$$

where the local z -axis is taken along the $\Gamma - L$ direction and the local x -axis along the $L - K$ direction in the Brillouin zone. Notice that these direction rotate with respect to the global coordinates from one L point to another. At the Weyl nodes, there is a degeneracy among two states with opposite symmetry under inversion. The physics of the two state system is captured by the σ matrices. Define q_{0z} and $\vec{q}_{0\perp}$ as the displacements of the node away from the L point parallel and perpendicular to the $\Gamma - L$ line respectively. θ is defined as the angle $\vec{q}_{0\perp}$ makes with the x -axis. The nodes are located at $\theta = p\pi/3$, $q_{0z} = \pm c_1 q_{0\perp}^3 / \beta$ (positive(negative) for odd (even) values of p), and $q_{0\perp}$ satisfying the equation $\Delta + q_{0z}^2/2m_1 - q_{0\perp}^2/2m_2 = 0$.

In the vicinity of these nodes the Hamiltonian can be expanded and written as

$$H_i(\delta\vec{q}) \approx \delta\vec{q} \cdot \mathbf{V}_i \cdot \vec{\sigma} \quad (2)$$

where $\delta\vec{q} = \vec{q} - \vec{q}_0$, and \mathbf{V}_i is a real matrix whose entries depend on the node index i . For the Hamiltonian in eq.1 the matrix \mathbf{V} is generically not symmetric and does not have all real eigenvalues. This is quite unlike the case considered in the context of the ABJ anomaly[16] or the anomalous hall effect [15]. For a diagonal \mathbf{V} matrix, the direction of the momentum, whose magnitude determines the energy if the lowest Landau level, is parallel to the applied magnetic field. Since momentum does not commute with the electromagnetic vector potential, and the fact that the latter is always transverse to the \vec{B} field, suggest that this property is generally valid. To understand the nature of the ABJ anomaly in iridates, we first verify that this conjecture holds for arbitrary \mathbf{V} matrices.

The procedure for computing the energy is sketched out here (details provided elsewhere [17]). Consider a single Weyl node in an applied magnetic field, \vec{B} . We can always rotate the coordinate system so that the \vec{B} lies in the xz -plane. In this reference frame $\vec{B} = B \{\sin(\theta), 0, \cos(\theta)\}$. Using a Landau gauge we write the corresponding vector potential as $B \{-\cos(\theta)y, 0, \sin(\theta)y\}$. Given this choice, the system is translationally invariant in the x and z directions. The wave-function of the LLL has the form $\{u, v\} \phi(y) e^{-i\delta k_x x - i\delta k_z z}$, where u and v are constants. Rather remarkable, the energy ϵ_0 , calculated with this choice of gauge, can be written in a gauge invariant form as

$$\epsilon_0 = - \frac{Det[\mathbf{V}]}{\|adj[\mathbf{V}] \cdot \vec{B}\|} \delta\vec{q} \cdot \vec{B} \quad (3)$$

where $Det[\mathbf{V}]$ and $adj[\mathbf{V}]$ are the determinant and adjugate of the matrix $[\mathbf{V}]$. The sign of the dispersion, and hence the chirality, is determined by the determinant. The energy is inversely proportional to the projection of the deviation of the momentum in the direction of the applied field.

An important point to note is that the energy depends on the full matrix \mathbf{V} and not just its determinant. Applying to graphene in a perpendicular magnetic field, it is easy to see that the energy is identically zero. The momentum is in-plane and has no projection along the applied field. For isotropic Weyl fermions where $\mathbf{V} = \pm v_f \mathbf{I}$, \mathbf{I} being the identity matrix, the dispersion reduces to $\pm v_f \delta\vec{q} \cdot \vec{B}$. If \mathbf{V} is diagonal but anisotropic, the units of length can be rescaled to bring the system back to an isotropic form [15]. In general the only statement that can be made is that the mode disperses only in the direction of the applied field, while the actual velocity cannot be determined without a detailed evaluation of the denominator in eqn.3.

Let us now consider the case of the pyrochlore iridates. Given the Hamiltonian (eqn.1) we can construct the relevant matrices. Since the different Weyl nodes in the iridates have different \mathbf{V} , all constructed with respect to their own local coordinate system, a general solution is prohibitive. To make further progress we use parameters that best fit the LSDA+U+SO calculations [10, 15]: $m_1 = m_2 = 0.5 \text{ eV}^{-1}$, $c_1 = c_2 = 1.0 \text{ eV}$, $\beta = 0.5 \text{ eV}$, $\Delta = 0.18 \text{ eV}$ (\vec{q} is dimensionless). These parameters give $q_{0\perp} = 0.48$ and $q_{0z} = \pm 0.22$.

To get insight on the general properties let us look at the nodes near [111]. The matrices for $\theta = \{0, 2\pi/3, -2\pi/3\}$ are

$$\mathbf{V}_{\theta=0} = \begin{pmatrix} 0 & 3q_{0\perp}^2 & -2q_{0\perp} \\ 3q_{0\perp}^2 & 0 & 0 \\ 0 & \frac{1}{2} & 2q_{0z} \end{pmatrix} \quad (4)$$

$$\mathbf{V}_{\theta=\pm 2\pi/3} = \begin{pmatrix} \mp \frac{3\sqrt{3}}{2} q_{0\perp}^2 & -\frac{3}{2} q_{0\perp}^2 & q_{0\perp} \\ -\frac{3}{2} q_{0\perp}^2 & \pm \frac{3\sqrt{3}}{2} q_{0\perp}^2 & \mp \sqrt{3} q_{0\perp} \\ 0 & \frac{1}{2} & 2q_{0z} \end{pmatrix}$$

Since the system possesses three fold rotation symmetry about the $\Gamma - L$ axis, these matrices are related by 120 degree rotation about the z -axis. If \mathbf{U} is a rotation matrix for $2\pi/3$ rotation about the local z -axis, than $\mathbf{U}\mathbf{V}_{\theta=0} = \mathbf{V}_{\theta=2\pi/3}$, $\mathbf{U}\mathbf{V}_{\theta=2\pi/3} = \mathbf{V}_{\theta=-2\pi/3}$ and $\mathbf{U}\mathbf{V}_{\theta=-2\pi/3} = \mathbf{V}_{\theta=0}$. In other words, knowing one is sufficient to generate the others. The determinant of these three matrices are all equal and given by $Det[\mathbf{V}]_i = -3q_{0\perp}^3 - 18q_{0\perp}^4 q_{0z}$.

The adjugate of a matrix \mathbf{V} is the transpose of the matrix of the cofactors of \mathbf{V} . The adjugates corresponding to those in eqn.4 are

$$\begin{aligned}
adj[\mathbf{V}_{\theta=0}] &= \begin{pmatrix} 0 & -6q_{0\perp}^2 q_{0z} - q_{0\perp} & 0 \\ -6q_{0\perp}^2 q_{0z} & 0 & -6q_{0\perp}^3 \\ \frac{3}{2}q_{0\perp}^2 & 0 & -9q_{0\perp}^4 \end{pmatrix} \\
adj[\mathbf{V}_{\theta=\pm 2\pi/3}] &= \begin{pmatrix} \pm \frac{\sqrt{3}}{2} (q_{0\perp} + 6q_{0\perp}^2 q_{0z}) & \frac{1}{2} (q_{0\perp} + 6q_{0\perp}^2 q_{0z}) & 0 \\ 3q_{0\perp}^2 q_{0z} & \mp 3\sqrt{3}q_{0\perp}^2 q_{0z} & -6q_{0\perp}^3 \\ -\frac{3}{4}q_{0\perp}^2 & \pm \frac{3\sqrt{3}}{4}q_{0\perp}^2 & -9q_{0\perp}^4 \end{pmatrix}
\end{aligned} \tag{5}$$

The adjugate matrices also respect a rotation properties about the z -axis. In this case we find $adj[\mathbf{V}]_{\theta=0} \mathbf{U}^\dagger = adj[\mathbf{V}]_{\theta=2\pi/3}$, $adj[\mathbf{V}]_{\theta=2\pi/3} \mathbf{U}^\dagger = adj[\mathbf{V}]_{\theta=4\pi/3}$ and $adj[\mathbf{V}]_{\theta=4\pi/3} \mathbf{U}^\dagger = adj[\mathbf{V}]_{\theta=0}$. Thus, unlike the Hamiltonian, the adjugates satisfy a right multiplication property.

We can construct all other matrices by symmetry. The matrices for the Weyl points related by inversion to those near [111] are obtained by changing the sign of the third column or equivalently the sign of σ_z . This remains true for all nodes related by inversion as the local z -axis changes sign. The nodes near $[\bar{1}\bar{1}1]$ have the same structure as those near [111] while those near $[\bar{1}1\bar{1}]$ have the sign of the first column changed. This ensures the geometry and helicity obtained within LSDA+U+SO calculations [10]. Given that the adjugate matrices are different at different nodes, we expect the response to a magnetic field to be highly anisotropic. To explore this further we turn to the magneto-conductivity.

Since the dispersion of the LLL is in the direction of the applied magnetic field, only the response to an electric field, $\vec{E} = E_0 \hat{B}$ applied parallel to the magnetic field will be considered. We will assume that the magnetic field is strong enough so that only the LLL is occupied. The dispersion being linear, elastic scattering within a single node is suppressed due to the lack of phase space. Stated differently no momentum relaxation is possible within a node. However the scattering between two nodes cannot be ignored. In fact, scattering between cones of opposite chirality is necessitated by the ABJ anomaly. In the presence of the electric field, there is a generation of RH particles and annihilation of LH particles. The rate of production is given by $\dot{N}_{||} = \delta q e B / \hbar = e^2 E_0 B / \hbar$, where eB/\hbar is the degeneracy of the LLL and $\delta q_{||}$ is the component of the momentum parallel to the magnetic field. This rate has to be balanced by the scattering between nodes with the opposite chirality to maintain a steady state.

Weyl nodes always come in pairs with opposite chirality. Before considering all 24 Weyl nodes, we first look at a single pair whose energies are given by $\epsilon_0 = \pm v \delta q_{||}$. For impurity scatterers, where the transition probability between states with different moment is independent of their momenta, the scattering rate, τ^{-1} is proportional

to the density of states and is given by

$$\frac{1}{\tau} = C \frac{eB}{v\hbar} \tag{6}$$

where C is a constant determined by the strength of scattering potential. We will comment on more general forms of scattering later. The ABJ anomaly requires an imbalance in particle number at the RH and LH Weyl nodes. If the difference in chemical potential between the RH and LH nodes is $\Delta\mu$, than energy balance requires

$$\Delta\mu = eE_0 v \tau \tag{7}$$

This is because over the scattering time τ , the momentum changes by $eE_0\tau$. Since the change in energy is v times change in momentum, the net energy transferred from one cone to the other is $eE_0\tau v$. A steady state is achieved if this transfer is balanced by the difference in chemical potential.

The difference in chemical potential leads to a current given by

$$\begin{aligned}
J_A &= e(eB/\hbar)\Delta\mu \\
&= e(eB/\hbar)eE_0 v \tau \\
&= C^{-1} e^2 v^2 E_0
\end{aligned} \tag{8}$$

The subscript A refers to the anomalous response. So far we have only considered momentum independent scattering rate. Let us look at the response in the presence of screened charged impurities characterized by matrix elements of the form $C/(q^2 + \kappa^2)$. The internode scattering probes intermediate to large momenta, as the nodes are physically separated in the Brillouin zone. The transition probabilities, which are proportional to the square of the matrix elements, fall off as $C/|\vec{q}|^4$ giving a large τ . In contrast, the conductivity in zero magnetic field is much smaller as it is dominated by intra-node scattering ($\sim C/\kappa^4$). Thus the conductivity in the presence of the magnetic field can be much larger than that in zero field. The results in eq.7 and eq.8, and the argument of large magnetoconductance, are the main conclusions of Nielsen and Ninomeya [16].

Having established the expected nature of the magneto-conductance, we return to the discussion of the iridates. The key feature of eq.8 is its dependence on the velocity v . As we have seen in our discussion of the dispersion of the LLL, the velocity can be tuned by changing the direction of the applied field. Moreover the different Weyl nodes have different Fermi wave-vector and different density of states. We will exploit the fact that the nodes always come in pairs and generalize the formulas derived above. We focus on three orientations of the applied field and assume that the dominant scattering is among nodes related by inversion.

(1) *Magnetic field along a principle axis (say z):* All the nodes on the $\Gamma - L - K$ plane have the same dispersion of the LLL. For the parameters specified above, the energy is $\epsilon_0 \approx \pm 0.14 \delta \vec{p} \cdot \hat{B}$, where the sign is determined by the chirality. All other nodes have $\epsilon_0 \approx \pm 0.38 \delta \vec{p} \cdot \hat{B}$. The velocity of low energy fermions differ by almost a factor of 3. Labeling the velocities as $v_1 = 0.14$ and $v_2 = 0.38$ the anomalous current generated is

$$\begin{aligned} J_A^1 &= C^{-1} e^2 (8v_1^2 + 16v_2^2) E_0 \\ &= 2.47 C^{-1} e^2 E_0 \end{aligned} \quad (9)$$

(2) *Magnetic field along $\Gamma - L$ (say $[111]$):* For this case the nodes divide into three categories. The six Weyl points that are in the vicinity of $[111]$ have the same velocity given by $v_1 = \pm 0.15$. At the other six equivalent L points, the three Weyl nodes split into one with velocity $v_2 = \pm 0.68$ and two with velocity $v_3 = \pm 0.24$. The larger value is associated with the node whose \vec{q}_0 's have a positive projection along the magnetic field. The anomalous current is

$$\begin{aligned} J_A^2 &= C^{-1} e^2 (6v_1^2 + 6v_2^2 + 12v_3^2) E_0 \\ &= 3.60 C^{-1} e^2 E_0 \end{aligned} \quad (10)$$

(3) *Magnetic field along $\Gamma - K$ (say $[110]$):* The nodes again split into three groups. There are four with velocity $v_1 = 0.69$ corresponding to the nodes which live in the $\Gamma - L - K$ plane perpendicular to the magnetic field. The other eight nodes close to these four have the same velocity of $v_2 = 0.3$. The four nodes in the $\Gamma - L - K$ plane containing the magnetic field have $v_2 = 0.3$ and the remaining eight have $v_3 = 0.15$.

$$\begin{aligned} J_A^3 &= C^{-1} e^2 (4v_1^2 + 12v_2^2 + 8v_3^2) E_0 \\ &= 3.16 C^{-1} e^2 E_0 \end{aligned} \quad (11)$$

It is clear from eqns. 9, 10 and 11 the proposed band structure of pyrochlore iridates leads to an anisotropic magneto-conductivity. In particular the anisotropy, defined as the difference in conductivity divided by the sum $(J_A^2 - J_A^1) / (J_A^2 + J_A^1)$, is as large as 19% between a field along a principal axis and one along $\Gamma - L$.

In analyzing the results of the three cases considered, we find that the density of states are almost equal. Thus thermodynamic properties such as specific heat are not as sensitive to the dependence of the dispersion on the magnetic field (in particular its direction). The fact that the anomalous production of Weyl fermions leads to a current that depends on the velocity provides a clear signature of the novel semi-metallic state. If one relaxes the assumption of scattering only between nodes related by inversion, than τ is a constant since the density of states does not change. In this case the current is proportional to sum of the absolute velocities of the nodes and the anisotropy is reduced to 5%. The presence of topologically protected surface states connect bulk nodes in pairs providing a mechanism for the transfer of Weyl particles[10]. How the surface states and the nature of scattering affect the anisotropy will be the subject of a future study.

In this letter we have considered the nature of magneto-conductance in Weyl semi-metals. In the presence of an applied field the energy of the LLL is obtained. We find that the level always disperses linearly with respect to the momenta parallel to the applied field. This result is general and holds even for systems with arbitrary Weyl hamiltonians. On the other hand the velocity of the low energy modes depends on the direction of the applied field. This feature is exploited in the context of the pyrochlore iridates. Using the symmetries of the crystal, we derive the Weyl equation at the 24 nodes. Applying magnetic fields in different directions allows us to manipulate the low energy physics, leading to anisotropic transport properties.

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